

Custodial $SO(4)$ symmetry and CP violation in N-Higgs-doublet potentials

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We study the implementation of global $SO(4) \sim SU(2)_L \otimes SU(2)_R$ symmetry in general potentials with N-Higgs-doublets in order to obtain models with custodial $SO(3)_C$ symmetry. We conclude that any implementation of the custodial $SO(4)$ symmetry is equivalent, by a basis transformation, to a canonical one if $SU(2)_L$ is the gauge factor, $U(1)_Y$ is embedded in $SU(2)_R$ and we require N copies of the doublet representation of $SU(2)_R$. The invariance by $SO(4)$ automatically leads to a CP-invariant potential and the basis of the canonical implementation of $SO(4)$ is aligned to a basis where CP symmetry acts in the standard fashion. We show different but equivalent implementations for the 2-Higgs-doublets model, including an implementation not previously considered.

I. INTRODUCTION

Despite the enormous success of the Standard Model of Particle Physics (SM) in accounting for all the known experimental data on high energy physics to date, several theoretical and observational ingredients pressure the SM for extensions. One can list naturalness problems such as the hierarchy problem or observational facts such as the need for new sources of CP violation, the need for nonordinary weakly interacting stable matter (dark matter) or a natural explanation for the smallness of nonzero neutrino masses.

The simplicity of the scalar sector of the SM, however, has some unique features owing to its minimality. Because of the presence of one Higgs doublet, the Higgs potential possesses a global accidental $SO(4)$ symmetry larger than the usual electroweak (EW) gauge symmetry $SU(2) \otimes U(1)_Y$ [1]. Even after electroweak symmetry breaking (EWSB), through the only symmetry breaking pattern, the $SO(3)_C$ portion of the global symmetry, usually called custodial symmetry [2–4], remains in the potential. The symmetry is only approximate because it is respected by the gauge interactions only in the $g_Y \rightarrow 0$ limit and by the Yukawa interactions only if the quarks in the same doublet have degenerate masses (it is then related to isospin symmetry). Nevertheless, such approximate symmetry guarantees the gauge bosons W_a^μ transform as a triplet of $SO(3)_C$ in the $g_Y \rightarrow 0$ limit and explains the absence of large radiative corrections to the ρ parameter from its tree-level value $\rho^{(0)} = M_W^2/M_Z^2 \cos^2 \theta_w = 1$, hence the name custodial symmetry.

When we try to extend the SM, the most simple extensions of the SM consider some enlargement of the scalar sector of the theory since it is the least verified sector either because the only elementary scalar of SM, the physical Higgs boson, has escaped discovery so far or we have had no final confirmation about the mechanism behind EWSB [5] and the origin of all the masses of the elementary particles of the SM. The simplest way to extend the scalar sector is to consider the replication of the Higgs doublet, leading to the N-Higgs-doublet models (NHDMs). The minimal version called 2-Higgs-doublets model (2HDM), was originally considered to implement the spontaneous CP violation mechanism [6], and more recently as simple extensions to address problems such as the little hierarchy problem [8], the presence and stability of dark matter candidates [7, 8], and to provide new sources of CP violation when extended to a 3HDM [9]. This model has also been extensively studied in the last years as the effective scalar sector of the MSSM [10–12]. For example, Ref. 10 presents a detailed study of the effective 2HDM potential that arises in the MSSM with explicit CP violation, after including radiative corrections.

Another reason to study this type of model is the presence of a horizontal space formed by the N -Higgs-doublets that possess the same gauge quantum numbers. An $SU(N)_H$ transformation in such space, then, only amounts to a reparametrization of the potential [13–17]. At the same time that the presence of a horizontal space makes the model more complex and less predictable due to the profusion of allowed couplings it also allows the study of the potential and its possible symmetry breaking patterns through the study of the orbit space of the gauge invariants [18–21].

In the NHDM extensions, with $N > 1$, the global $SO(4)$ symmetry does not arise naturally as an accidental symmetry but has to be imposed. Once it is imposed and leads to the custodial symmetry $SO(3)_C$, it can play its original role to protect large radiative corrections to the ρ parameter [22–25]. In the context of the 2HDM, the global

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$SO(4)$ symmetry leads to the degeneracy of the charged scalar and one of the neutral scalars [26]. In one version [23], it is possible to construct a 2HDM model with custodial symmetry such that the state degenerate to the charged Higgs is a CP-even neutral Higgs, $M_{H^0} = M_{H^\pm}$, instead of the more usual $M_{A^0} = M_{H^\pm}$ scenario.

We intend to consider here the NHDM extensions of the SM possessing the custodial $SO(4)$ symmetry which, in turn, can be broken down to the custodial $SO(3)_C$ symmetry that protects the ρ parameter. Larger global symmetries can be considered [27] but in general it will produce more pseudo-Goldstone bosons [28] in addition to the usual three would-be Goldstone bosons absorbed by the Higgs mechanism. We can separate our goals in this study into two categories: construction and identification. The first refers to the construction of general custodial invariant NHDM potentials and analysis of the models. The second goal refers to the methods of identifying the $SO(4)$ symmetry if it is not manifest and concealed such as the CP symmetry acting in a general basis [13, 14, 17]. It is then important to study the interplay between the imposition of $SO(4)$ symmetry and the reparametrization group $SU(N)_H$. In particular, it is important to emphasize that the global $SO(4)$ symmetry, like CP symmetry, is not contained in $SU(2)_L \otimes U(1)_Y \otimes SU(N)_H$ as most of the symmetries usually considered for NHDMs are. See, for instance, the symmetries for 2HDM and 3HDM in Refs. [20, 21, 29]. The analysis of basis transformations is also crucial when extending some symmetries of the potential to the Yukawa interactions, since some symmetries of the potential might be broken by the Yukawa terms as well as the converse [22, 24, 30, 31].

In the context of the 2HDM, many studies [22, 24, 25] show that CP invariance and custodial symmetry are intimately connected. In fact, we will see that such connection can be extended to general custodial-invariant NHDMs. In certain cases the knowledge of the presence of the CP symmetry and how it acts on the fields, allows us to infer if $SO(4)$ is also present as a symmetry. We can also borrow the various methods of identifying CP invariance independently of the basis [13, 15, 17]. Compared to the SM, where global $SO(4)$ symmetry, custodial $SO(3)_C$ symmetry and CP symmetry are automatic in the scalar sector, we will see that a NHDM potential invariant by $SO(4)$ symmetry and a potential invariant by CP symmetry differ only minimally in an easily identifiable manner for $N = 2$ and $N = 3$ Higgs doublets. For $N \geq 4$, a custodial-invariant potential is also more constrained than a CP-invariant potential but the difference is more involved.

The paper is organized as follows: In Sec. II we study one particular implementation of the global custodial $SO(4)$ symmetry called canonical implementation and how it is related to the CP symmetry and basis transformations. In particular, in Sec. IID we show any implementation of the global symmetry $SO(4)$ is equivalent to the canonical implementation. Section III shows the various implementations for the 2HDM considered in the literature, shows their equivalence to the canonical implementation and also shows one different but equivalent implementation. We discuss some consequences of this work in Sec. IV, followed by the conclusions. To clarify the nomenclature regarding the various groups involved in the study of the custodial symmetry, e.g., $SO(3)$, $SO(4)$ and $SU(2)_L \otimes SU(2)_R$, we refer to Appendix A, where we list the group/subgroup structure of the global symmetries involved in the SM. Instead of distinguishing the various (custodial) symmetries by names, we will denote them by their group structure and use the isomorphic groups interchangeably, often considering their local structure only. We will often include a subscript “C” (custodial) to denote the groups, as in $SO(4)_C$.

II. CANONICAL IMPLEMENTATION OF $SO(4)_C$ IN NHDM

Let us consider N Higgs-doublets of $SU(2)_L$ of hypercharge $Y = 1$: ϕ_a , $a = 1, \dots, N$.

Let us also define a 2×2 complex matrix of fields [4, 5]

$$\Phi_a \equiv (\tilde{\phi}_a | \phi_a) = \begin{pmatrix} \phi_a^{0*} & \phi_a^+ \\ -\phi_a^- & \phi_a^0 \end{pmatrix}, \quad (1)$$

where $\tilde{\phi}_a \equiv \epsilon \phi_a^*$ ($\epsilon \equiv i\sigma_2$) defines the tilde ($\tilde{}$) operation on a doublet which transforms a $Y = 1$ doublet to a $Y = -1$ doublet. We can also define the ($\tilde{}$) operation on any 2×2 complex matrix h as

$$\tilde{h} \equiv \epsilon h^* \epsilon^\dagger. \quad (2)$$

It is straightforward to see that such operation is trivial on Φ_a of Eq. (1), i.e.,

$$\tilde{\Phi}_a = \Phi_a. \quad (3)$$

We can define the Canonical Implementation (CI) of the custodial group $SU(2)_L \otimes SU(2)_R$ by the universal action upon Φ_a , $a = 1, \dots, N$,

$$\Phi_a \rightarrow U_L \Phi_a U_R^\dagger, \quad U_L \in SU(2)_L \text{ and } U_R \in SU(2)_R. \quad (4)$$

The action (4) sets the representation of Φ_a as $(2, 2)$ under the custodial group $SU(2)_L \otimes SU(2)_R$. Therefore, each Higgs-doublet ϕ_a has the same transformation property under $SU(2)_L \otimes SU(2)_R$ as the SM Higgs-doublet.

Within this section we will focus on the canonical implementation of the custodial group $SO(4)_C$ and any mention to the custodial group will denote this implementation. Within the 2-Higgs-doublet model, this implementation was named type I in an early work [22].

It is clear that the identity (3) preserves the action (4) since

$$\epsilon U^* \epsilon^\dagger = U, \quad \text{for any } U \in SU(2).$$

Using the operation (2) we can write the previous identity as

$$\tilde{U} = U, \quad \text{for any } U \in SU(2). \quad (5)$$

If the transformation (4) is promoted to a symmetry of the N -Higgs-doublet potential, we say the potential is *custodial-invariant*. As in the SM, such symmetry is explicitly broken by the gauge interactions that are invariant only by the gauged $SU(2)_L \otimes U(1)_Y$ subgroup. In the usual EWSB scenario, the three would-be Goldstone bosons that appear in the breaking of $SU(2)_L \otimes SU(2)_R \rightarrow SU(2)_{L+R}$ coincide with the usual would-be Goldstone bosons of the breaking of $SU(2)_L \otimes U(1)_Y \rightarrow U(1)_{em}$. They are then absorbed as the longitudinal components of the gauge bosons W^\pm, Z^0 by the Higgs mechanism, such that no physical Goldstone bosons appear. Other symmetry-breaking patterns exist where physical pseudo-Goldstone bosons appear. That is the case of certain 2-Higgs-doublet potentials with global symmetries equal or larger than $SO(4)_C$ (see Sec. IIB and Ref. 27).

The correspondence between the representation $(2, 2)$ of $SU(2)_L \otimes SU(2)_R$ and the vector representation $\mathbf{4}$ of $SO(4)_C$ guarantees we can construct a 4-vector out of the real and imaginary parts of the two components of ϕ_a .

The usual correspondence is found by defining four real fields $\eta^{(a)} = (\eta_\mu^{(a)}) = (\eta_0^{(a)}, \boldsymbol{\eta}^{(a)})$, $\boldsymbol{\eta}^{(a)} = (\eta_1^{(a)}, \eta_2^{(a)}, \eta_3^{(a)})$, from the relation

$$\Phi_a = \eta^{(a)} \mathbb{1} + i \boldsymbol{\sigma} \cdot \boldsymbol{\eta}^{(a)} = \begin{pmatrix} \eta_0^{(a)} + i \eta_3^{(a)} & i \eta_1^{(a)} + \eta_2^{(a)} \\ i \eta_1^{(a)} - \eta_2^{(a)} & \eta_0^{(a)} - i \eta_3^{(a)} \end{pmatrix}. \quad (6)$$

We can rewrite (6) in a more compact form

$$\Phi_a = \eta_\mu^{(a)} \mathbf{e}_\mu, \quad (7)$$

by defining $(\mathbf{e}_\mu) \equiv (\mathbb{1}, i\sigma_1, i\sigma_2, i\sigma_3)$.

The custodial symmetry $SU(2)_L \otimes SU(2)_R$ acting as (4) induces in $\eta^{(a)}$ the transformations

$$\eta_\mu^{(a)} \rightarrow R_{\mu\nu}(U_L, U_R) \eta_\nu^{(a)}, \quad R(U_L, U_R) \in SO(4), \quad (8)$$

where the convention of summation of repeated indices is implicit for $\mu, \nu = 0, 1, 2, 3$. It can be shown that $R(U_L, U_R)$ defines a two-to-one mapping between $SU(2)_L \otimes SU(2)_R$ and $SO(4)_C$ with the explicit function

$$R_{\mu\nu}(U_L, U_R) \equiv \frac{1}{2} \text{Tr}[\mathbf{e}_\mu^\dagger U_L \mathbf{e}_\nu U_R^\dagger]. \quad (9)$$

Hence $\eta^{(a)}$ can be regarded as vectors in a four-dimensional euclidean space. We can also recover the $SU(2)_{L+R} \rightarrow SO(3)$ mapping for $U_R = U_L$ [17].

We can also define a 4-component complex vector (in a four-dimensional real vector space) that transforms more directly under $SU(2)_L \otimes SU(2)_R$. Let us define

$$\chi_a \equiv \begin{pmatrix} \phi_a \\ -\tilde{\phi}_a \end{pmatrix}. \quad (10)$$

The action (4) is then translated into

$$\chi_a \rightarrow U_R \otimes U_L \chi_a. \quad (11)$$

The transformation property (11) can be deduced if we rewrite (4) as $\Phi_{aij} \rightarrow U_{Lii'} U_{Rjj'}^* \Phi_{ai'j'}$ [note that $\chi_a = (\epsilon \otimes \mathbb{1}_2)(\Phi_{a11}, \Phi_{a21}, \Phi_{a12}, \Phi_{a22})^\top$ implies the transformation property $\chi_a \rightarrow (\epsilon \otimes \mathbb{1}_2)(U_R^* \otimes U_L)(\epsilon^\dagger \otimes \mathbb{1}_2)\chi_a$ and finally use the identity (5)].

One can also write explicitly the linear relation between χ_a and $\eta^{(a)}$ as

$$\chi_a = \mathcal{B} \eta^{(a)}, \quad (12)$$

where the transformation matrix \mathcal{B} can be read off from (6). With this change of basis it is possible to write explicitly how the generators of $SU(2)_L \otimes SU(2)_R$ acting on χ_a are related to the generators of $SO(4)_C$ acting on $\eta^{(a)}$. Such generators can be found in appendix B.

A. Custodial invariants and explicit CP invariance

For the construction of a renormalizable N-Higgs-doublet potential that is invariant by the custodial group $SO(4)_C$ in the canonical implementation (4), we need to identify the minimal custodial invariants.

The terms that are invariant by (4), up to mass order 4, are

$$\begin{aligned} \text{Tr}[\Phi_a^\dagger \Phi_b] &= \phi_a^\dagger \phi_b + h.c., \\ \text{Tr}[(\Phi_a^\dagger \Phi_b)(\Phi_c^\dagger \Phi_d)] &= \phi_a^\dagger \phi_b \phi_c^\dagger \phi_d - \phi_a^\dagger \phi_c \phi_b^\dagger \phi_d + \phi_a^\dagger \phi_d \phi_b^\dagger \phi_c \\ &\quad + h.c. \end{aligned} \quad (13)$$

It was necessary to use some reordering identities such as $\phi_a^\dagger \tilde{\phi}_b \tilde{\phi}_c^\dagger \phi_d = \phi_a^\dagger \phi_d \phi_b^\dagger \phi_c - \phi_a^\dagger \phi_c \phi_b^\dagger \phi_d$ by making use of the identity $\epsilon_{ij}\epsilon_{kl} = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}$. There are no other invariants of the same orders and apparently independent invariants are reducible to the ones in Eq. (13). For instance, $\det \Phi_a = \frac{1}{2} \text{Tr}[\Phi_a^\dagger \Phi_a]$, and $\epsilon_{ii'}\epsilon_{jj'}\Phi_{a ij}\Phi_{b i' j'} = \frac{1}{2} \text{Tr}[\Phi_a^\dagger \Phi_b]$, due to (3).

We immediately notice that the custodial invariants (13) are invariant by the canonical CP (CCP) transformations

$$\phi_a(x_0, \mathbf{x}) \xrightarrow{\text{CCP}} \phi_a^*(x_0, -\mathbf{x}), \quad a = 1, \dots, N. \quad (14)$$

Such transformations act linearly upon χ_a (10) as

$$\chi_a \xrightarrow{\text{CCP}} \begin{pmatrix} 0 & \epsilon \\ -\epsilon & 0 \end{pmatrix} \chi_a, \quad (15)$$

and upon $\eta^{(a)}$ (6) as

$$(\eta_0^{(a)}, \eta_1^{(a)}, \eta_2^{(a)}, \eta_3^{(a)}) \xrightarrow{\text{CCP}} (\eta_0^{(a)}, -\eta_1^{(a)}, \eta_2^{(a)}, -\eta_3^{(a)}). \quad (16)$$

We realize that $\eta_0^{(a)}, \eta_2^{(a)}$ are CP-even fields while $\eta_1^{(a)}, \eta_3^{(a)}$ are CP-odd fields. Such transformation is in accordance with $\Phi_a \rightarrow \Phi_a^* = \epsilon \Phi_a \epsilon^\dagger$.

Since any custodial-invariant potential can be written as functions of the basic custodial invariants (13), we can conclude that *a N-Higgs-doublet potential which is invariant by the custodial group $SO(4)_C$ in its canonical form (4) is automatically explicitly CP-invariant in its canonical form (14)*. This result was established in Ref. 22 for the 2HDM potential considering the canonical implementation (type I) as well as a different implementation named type II. The latter, in fact, can be shown to be equivalent to the canonical implementation in a different basis [24, 25]. We will discuss basis transformations in Sec. II C and show in Sec. II D that any implementation of $SO(4)_C$ in a NHDM potential is equivalent to the canonical implementation in some basis.

We can ask the converse: Is an explicitly CP invariant NHDM potential automatically invariant by the custodial group $SO(4)_C$? We know from the 2HDM potential [22, 24, 25] that the answer is negative. The immediate following question is: what additional feature makes a CP-invariant potential also custodial-invariant? We will show in the following, within the canonical implementation, that the additional condition is minimal for $N \leq 3$. The characterization for $N \geq 4$ will be seen to be more involved.

For the 2HDM potential, the relation between custodial invariance and CP symmetry was already explored in Refs. [24, 25]. When basis transformations are allowed, such a relation can be related to the existence of a basis where the implementation of both the custodial group $SO(4)_C$ and the CP symmetry are the canonical ones. We will generalize this notion to general N-Higgs-doublets.

To distinguish between a NHDM potential invariant by the CCP (14) and by the custodial group $SO(4)_C$ (4) we need to analyze the terms allowed by each symmetry to appear in a general potential.

We know the most general renormalizable NHDM potential can be written in terms of the linear and quadratic combinations of the minimal gauge invariants [17]

$$\phi_a^\dagger \phi_b, \quad a, b = 1, \dots, N. \quad (17)$$

Only $4N - 4$ of them are algebraically independent [19] when the fields are considered as c-numbers. This fact affects the minimization procedure.

Instead of working with complex quantities, we can consider the equivalent set of real quantities

$$\begin{aligned} \text{Re}(\phi_a^\dagger \phi_b), & \quad a \leq b = 1, \dots, N, \\ \text{Im}(\phi_a^\dagger \phi_b), & \quad a < b = 2, \dots, N. \end{aligned} \quad (18)$$

If we succeed in writing the gauge invariants (18) in terms of the custodial invariants (13), then we can write a general custodial invariant potential.

For the terms of mass order 2, we can check the correspondence is

$$\text{Re}(\phi_a^\dagger \phi_b) = \frac{1}{2} \text{Tr}[\Phi_a^\dagger \Phi_b], \quad a \leq b = 1, \dots, N, \quad (19)$$

$$\text{Im}(\phi_a^\dagger \phi_b) = \frac{i}{2} \text{Tr}[\Phi_a^\dagger \Phi_b \sigma_3], \quad a < b = 2, \dots, N. \quad (20)$$

The term (20), however, is not custodial-invariant but transforms as the third component of a vector $\mathbf{z}_{ab} = (z_{ab}^A)$ of $SU(2)_R$ defined as

$$z_{ab}^A \equiv \frac{i}{2} \text{Tr}[\Phi_a^\dagger \Phi_b \sigma_A], \quad A = 1, 2, 3. \quad (21)$$

In fact, the components 1 and 2 of $\mathbf{z}_{ab} = (z_{ab}^A)$ are not $U(1)_Y$ invariants as

$$z_{ab}^1 = \text{Im}(\phi_a^\dagger \epsilon \phi_b), \quad z_{ab}^2 = \text{Re}(\phi_a^\dagger \epsilon \phi_b). \quad (22)$$

Notice $\mathbf{z}_{aa} = \mathbf{0}$ and there is no such term in the SM ($N = 1$).

Both custodial invariance and CCP symmetry forbid any terms of the form below in the potential:

$$\text{Im}(\phi_a^\dagger \phi_b), \quad a < b = 2, \dots, N, \quad (23)$$

$$\text{Re}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d), \quad a \leq b = 1, \dots, N, \quad c < d = 2, \dots, N, \quad (24)$$

On the other hand, both custodial invariance and CCP symmetry allow the terms

$$\text{Re}(\phi_a^\dagger \phi_b), \quad a \leq b = 1, \dots, N, \quad (25)$$

$$\text{Re}(\phi_a^\dagger \phi_b) \text{Re}(\phi_c^\dagger \phi_d), \quad a \leq b = 1, \dots, N, \quad c \leq d = 1, \dots, N. \quad (26)$$

The only missing fourth-order terms are CCP-invariant but not custodial-invariant. They are

$$\text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d), \quad a < b = 2, \dots, N, \quad c < d = 2, \dots, N. \quad (27)$$

However, if combined with other terms as

$$\mathbf{z}_{ab} \cdot \mathbf{z}_{cd} = \text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d) + \text{Re}(-\phi_a^\dagger \phi_d \phi_b^\dagger \phi_c + \phi_a^\dagger \phi_c \phi_b^\dagger \phi_d), \quad (28)$$

it becomes custodial-invariant. This term is contained in the second expression of (13) since

$$\frac{1}{2} \text{Tr}[(\Phi_a^\dagger \Phi_b)(\Phi_c^\dagger \Phi_d)] = \text{Re}(\phi_a^\dagger \phi_b) \text{Re}(\phi_c^\dagger \phi_d) - \mathbf{z}_{ab} \cdot \mathbf{z}_{cd}. \quad (29)$$

Considering the properties $\mathbf{z}_{ba} = -\mathbf{z}_{ab}$ and $\mathbf{z}_{aa} = \mathbf{0}$, we note that if some of the indices of (28) are equal, excluding $a = b$ or $c = d$, the term $\text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d)$ is effectively canceled out. For example, for $b = c$,

$$\mathbf{z}_{ab} \cdot \mathbf{z}_{bd} = \text{Re}(\phi_a^\dagger \phi_b) \text{Re}(\phi_b^\dagger \phi_d) - \phi_b^\dagger \phi_b \text{Re}(\phi_a^\dagger \phi_d). \quad (30)$$

Hence terms $\mathbf{z}_{ab} \cdot \mathbf{z}_{cd}$ with two equal indices do not generate new genuine fourth-order custodial invariants besides the product of two quadratic invariants.

The property (30) means that custodial-invariant potentials with $N = 2$ and $N = 3$ Higgs doublets do not contain terms of the form $\text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d)$. The custodial-invariant 2HDM in its canonical form is, in fact, equivalent to a CP-invariant (real) potential without the quartic term $\text{Im}^2(\phi_1^\dagger \phi_2)$ [24, 25, 27].

Therefore, we can state that *a NHDM potential, with $N \leq 3$, invariant by the custodial group $SO(4)_C$ in its canonical implementation (4) is equal to a potential invariant by CCP (14) with the additional elimination of terms of the form $\text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d)$.* From a CP-invariant potential in its real basis, the latter elimination corresponds to the elimination of one term for $N = 2$ and 6 terms for $N = 3$. In this case, it is straightforward to construct a general $SO(4)_C$ -invariant potential: only consider the terms in Eqs. (25) and (26). Such potential will have 9 and 27 real parameters for the 2HDM and 3HDM, respectively. [A total of $2 + 2(r + q) + (r + q)(r + q + 1)/2$ real parameters, where $r = N - 1$ and $q = N(N - 1)/2$.]

One important remark concerning the description above is that for the full quantum theory considering radiative corrections, since gauge interactions do not respect the full custodial group $SO(4)_C$, the effective potential will almost inevitably contain terms of the form $\text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d)$ generated by finite radiative corrections. But since CP

symmetry is a good symmetry of the potential and gauge interactions, the terms (23) and (24) can only be generated from other sectors that violate CP, such as Yukawa interactions.

For $N \geq 4$, the terms $\text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d)$ might be present in the potential contained in new genuine fourth order custodial invariants such as

$$\mathbf{z}_{12} \cdot \mathbf{z}_{34} = \text{Im}(\phi_1^\dagger \phi_2) \text{Im}(\phi_3^\dagger \phi_4) + \text{Re}(-\phi_1^\dagger \phi_4 \phi_2^\dagger \phi_3 + \phi_1^\dagger \phi_3 \phi_2^\dagger \phi_4). \quad (31)$$

We note, however, that the custodial invariants $\mathbf{z}_{ab} \cdot \mathbf{z}_{cd}$, with $a \neq b \neq c \neq d$, still contain quadratic combinations of second-order custodial invariants $\text{Re}(\phi_a^\dagger \phi_b)$, and we conclude they are reducible in some way. We are obviously interested in identifying the irreducible piece.

The irreducible fourth-order invariants can be constructed most easily by using the real components (6). We begin by rewriting the second-order invariants

$$\eta^{(a)} \cdot \eta^{(b)} = \frac{1}{2} \text{Tr}[\Phi_a^\dagger \Phi_b] = \text{Re}(\phi_a^\dagger \phi_b). \quad (32)$$

The only $SO(4)_C$ invariant that can be constructed out of four 4-vectors $\eta^{(a)}, \eta^{(b)}, \eta^{(c)}, \eta^{(d)}$ which is also independent of (32) is the pseudoscalar

$$I_{abcd}^{(4)} \equiv \epsilon_{\mu\nu\alpha\beta} \eta_\mu^{(a)} \eta_\nu^{(b)} \eta_\alpha^{(c)} \eta_\beta^{(d)}, \quad (33)$$

where the $\epsilon_{\mu\nu\alpha\beta}$ is the totally antisymmetric tensor in four dimensions obeying $\epsilon_{0123} = 1$. We could have also written $I_{abcd}^{(4)} = \det \eta^{(abcd)}$ for $\eta^{(abcd)} \equiv (\eta^{(a)} | \eta^{(b)} | \eta^{(c)} | \eta^{(d)})$ as a 4×4 matrix. The $SO(4)$ invariant (33) is the genuine custodial invariant that only appears for 4 or more vectors (doublets). If any two of the indices a, b, c, d are equal the invariant is null.

We can rewrite $I^{(4)}$ in terms of Higgs-doublets or \mathbf{z}_{ab} (21) as

$$I_{abcd}^{(4)} = \text{Im}(\phi_a^\dagger \phi_b) \text{Im}(\phi_c^\dagger \phi_d) + \text{Im}(\phi_a^\dagger \phi_d) \text{Im}(\phi_b^\dagger \phi_c) \\ + \text{Im}(\phi_a^\dagger \phi_c) \text{Im}(\phi_d^\dagger \phi_b), \quad (34)$$

$$= \mathbf{z}_{ab} \cdot \mathbf{z}_{cd} + \mathbf{z}_{ac} \cdot \mathbf{z}_{db} + \mathbf{z}_{ad} \cdot \mathbf{z}_{bc}. \quad (35)$$

We note that the imaginary parts of the gauge invariants $\text{Im}(\phi_a^\dagger \phi_b)$ only appear through the combination (34) since

$$\mathbf{z}_{ab} \cdot \mathbf{z}_{cd} = (\eta^{(a)} \cdot \eta^{(c)})(\eta^{(b)} \cdot \eta^{(d)}) - (\eta^{(a)} \cdot \eta^{(d)})(\eta^{(b)} \cdot \eta^{(c)}) \\ + I_{abcd}^{(4)}. \quad (36)$$

The invariant $I_{abcd}^{(4)}$ changes sign by exchange of any pair of indices among $(abcd)$ and hence by any odd permutation. An even permutation of $(abcd)$, on the other hand, leaves $I_{abcd}^{(4)}$ invariant. Thus each term $I_{abcd}^{(4)}$ is invariant by an $A_4 \subset SO(4)_H$ discrete symmetry in each horizontal subspace spanned by $\{\phi_a, \phi_b, \phi_c, \phi_d\}$.

Another useful formula is

$$\det(\text{Im} K^{(1234)}) = (I_{1234}^{(4)})^2, \quad (37)$$

where $K^{(1234)}$ is the submatrix of K , given by $K_{ab} = \phi_b^\dagger \phi_a$ [16, 19], constructed from the intersection of the rows 1,2,3,4 with columns 1,2,3,4.

Notice that the doublets live in the space \mathbb{C}^2 and then at most two doublets can be linearly independent. Instead, when we are transported to \mathbb{R}^4 through Eq. (6), four 4-vectors can be linearly independent, as they should be. For example, if $\phi_3 = \alpha \phi_1 + \beta \phi_2$ for ϕ_1, ϕ_2 linearly independent, then still $\{\eta^{(3)}, \eta^{(1)}, \eta^{(2)}\}$ is linearly independent if $\text{Im} \alpha \neq 0$ or $\text{Im} \beta \neq 0$.

For completeness, we can rewrite the $SU(2)_R$ vectors (21) as vectors of $SO(3)_C$:

$$\mathbf{z}_{ab} = \eta_0^{(a)} \boldsymbol{\eta}^{(b)} - \eta_0^{(b)} \boldsymbol{\eta}^{(a)} + \boldsymbol{\eta}^{(a)} \times \boldsymbol{\eta}^{(b)}. \quad (38)$$

The most general custodial invariant NHD potential for $N \geq 4$ can be written as the most general linear combination of terms of Eqs. (25), (26) and (34). For the invariants $I_{abcd}^{(4)}$, there is only one invariant for each set $(abcd)$ with all distinct indices. For example, for $N = 4$, we know there is only one invariant. For $N \geq 5$, there will be $\binom{N}{4}$ invariants.

To perform the minimization of the potential with $N \geq 5$, however, we need to know additionally how many invariants $I^{(4)}$ are functionally independent among the $\binom{N}{4}$ invariants.

B. Isotropy groups and symmetry breaking

Let us analyze here what are the possible symmetry groups that are left invariant when the N -Higgs-doublets acquire nonzero vacuum expectation values (VEVs), required from successful EWSB, in a potential invariant by the custodial group $SO(4)_C$. The VEVs are realized as the absolute minimum of the Higgs potential and their isotropy groups define the spontaneous symmetry-breaking pattern. The specific patterns depend on the parameters of the potential but one can study the maximal realizable symmetry-breaking patterns from the possible isotropy groups of general VEVs with respect to both $SO(4)_C$ (global) and $SU(2)_L \otimes U(1)_Y$ (gauge).

Let us begin with the custodial group and consider N Higgs-doublets ϕ_a , together with their corresponding natural forms Φ_a and $\eta^{(a)}$, upon which $SU(2)_L \otimes SU(2)_R$ and $SO(4)_C$ act naturally as in Eqs. (4) and (8) respectively. We want to study how the possible isotropy groups H_C change as N grows. We will assume that all $\langle \phi_a \rangle \neq \mathbf{0}$. Otherwise, it will coincide with the VEVs for smaller N . In any case, successful EWSB also requires $\sum_a \langle \phi_a^\dagger \phi_a \rangle = v_L^2/2$, where $v_L \sim 246\text{GeV}$.

For $N = 1$ Higgs doublet ϕ_1 (SM), $SO(4)_C$ is an automatic global symmetry of the Higgs potential and the custodial symmetry $SO(3)_C$ always remains in the potential after EWSB breaking because we can rotate away any corresponding VEV $\langle \Phi_1 \rangle$ by a global symmetry $SU(2)_L$ alone and obtain

$$\langle \Phi_1 \rangle = v_1 \mathbb{1}, \quad (39)$$

where $\sqrt{2}v_1 = 246\text{GeV}$ within the SM. The isotropy group is $H_C = SU(2)_{L+R} \sim SO(3)_C$. The VEV above automatically conserves CP. In terms of the real field $\eta^{(1)}$ it is also obvious that any VEV $\langle \eta^{(1)} \rangle = (v_1, 0, 0, 0)$ would leave an $SO(3)_C$ group invariant.

For $N = 2$ Higgs doublets ϕ_1, ϕ_2 , the global symmetry $SO(4)_C$ is not automatic and has to be imposed in the potential. But once it is imposed, CP is an automatic symmetry of the potential. If we consider that EWSB proceeds through the VEVs $\langle \Phi_1 \rangle \neq 0, \langle \Phi_2 \rangle \neq 0$, then we can rotate $\langle \Phi_1 \rangle$ to the form (39) by a global $SU(2)_L$ transformation. We can still apply an $SU(2)_{L+R}$ transformation [$U_R = U_L$ in Eq. (4)] which leaves $\langle \Phi_1 \rangle$ invariant but allows us to write

$$\langle \Phi_2 \rangle = v_2 e^{-i\varphi_2 \sigma_3}. \quad (40)$$

We have parametrized $\langle \eta^{(2)} \rangle = (v_2 \cos \varphi_2, 0, 0, -v_2 \sin \varphi_2)$ for convenience. If $\varphi_2 \neq 0, \pi$, the isotropy group left invariant by $\langle \Phi_1 \rangle$ and $\langle \Phi_2 \rangle$ in Eqs. (39) and (40) is $H_C = U(1)_{T_{3R}+T_{3R}} \sim SO(2)_C$.

For $N \geq 3$ Higgs doublets, the isotropy group can be reduced to the trivial $H_C = \{\mathbb{1}\}$ or some discrete group. If $\langle \Phi_1 \rangle, \langle \Phi_2 \rangle \neq 0$, we can rotate $\langle \Phi_1 \rangle, \langle \Phi_2 \rangle$ to the forms (39) and (40) through global transformations. For $\langle \Phi_3 \rangle \neq 0$, we can use the $U(1)_{T_{3R}+T_{3R}}$ freedom to write

$$\langle \Phi_3 \rangle = \langle \eta_0^{(3)} \rangle \mathbb{1} + \langle \eta_2^{(3)} \rangle i\sigma_2 + \langle \eta_3^{(3)} \rangle i\sigma_3. \quad (41)$$

If $\langle \eta_2^{(3)} \rangle \neq 0$, there is no continuous symmetry left and the isotropy group is $H_C = \{\mathbb{1}\}$ or some discrete group. For the nonzero VEVs $\langle \Phi_a \rangle$, $a \geq 4$, all the possible components are meaningful because there is no continuous symmetry.

In terms of the gauge group $SU(2)_L \otimes U(1)_Y$, the possible isotropy groups H for $N = 1, 2, 3, \dots$, are known. For $N = 1$, $H = U(1)_{em}$ and the conventional form for $\langle \phi_1 \rangle$ is

$$\langle \phi_1 \rangle = \begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \quad v_1 > 0. \quad (42)$$

It is the equivalent of Eq. (39) in terms of doublets.

For $N = 2$, we can preserve the form of (42). The isotropy group H is trivial if a_2 is nonzero for the general form

$$\langle \phi'_2 \rangle = v_2 \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}, \quad v_2 > 0, \quad a_2 \geq 0, \quad (43)$$

where b_2 is a nonzero complex number. For nonzero a_2 , this VEV corresponds to charge breaking vacuum (CB-V). This VEV contrasts to Eq. (40) whose doublet version is

$$\langle \phi_2 \rangle = v_2 \begin{pmatrix} 0 \\ e^{i\varphi_2} \end{pmatrix}, \quad v_2 > 0. \quad (44)$$

It corresponds to a vacuum that spontaneously breaks CP (CPB-V) in a real potential. In a general 2HDM potential, the VEVs (43) and (44) correspond to physically very different situations. In a custodial invariant potential, however, they are in the same $SO(4)_C$ stratum and have the same $SO(2)_C$ isotropy group with respect to $SO(4)_C$.

In fact, in a custodial-invariant potential, *a CPB vacuum and a CB vacuum are always degenerate at tree level*. In other words, if a VEV of the form (44) is a minimum of the potential, then there are infinite continuously related VEVs of the form (43) corresponding to the same minimum value of the potential. The reason is that $V(U_L \langle \Phi_1 \rangle U_R^\dagger, U_L \langle \Phi_2 \rangle U_R^\dagger) = V(\langle \Phi_1 \rangle, \langle \Phi_2 \rangle)$ and we can relate the matrices $\langle \Phi_a \rangle$ in Eqs. (39) and (40) to the following matrices through an $SU(2)_{L+R}$ transformation:

$$U_L \langle \Phi_1 \rangle U_R^\dagger = \langle \Phi_1 \rangle, \quad (45)$$

$$U_L \langle \Phi_2 \rangle U_R^\dagger = v_2 (\cos \varphi_2 \mathbb{1} - \sin \varphi_2 i \boldsymbol{\sigma} \cdot \mathbf{n}), \quad (46)$$

where $\mathbf{n} = (\sin \theta \cos \alpha, \sin \theta \sin \alpha, \cos \theta)$ and

$$U_L = U_R = e^{-i\sigma_3 \alpha/2} e^{-i\sigma_2 \theta/2}. \quad (47)$$

The VEV (46) corresponds to the form (43) if we associate $b_2 = \cos \varphi_2 + i \sin \varphi_2 \cos \theta$ and $a_2 = \sin \varphi_2 \sin \theta$ for $\alpha = 3\pi/2$ in Eq. (47).

Another way of looking into the degeneracy between a CPB vacuum and a CB vacuum is to analyze the basis invariant that signals CB [18]: $\langle r_0 \rangle^2 - |\langle \mathbf{r} \rangle|^2 \geq 0$. Only the equality signals a neutral vacuum. The variables r_μ , $\mu = 0, 1, \dots, N^2 - 1$ are linear combinations of $\phi_a^\dagger \phi_b$ (17) that will be properly defined in Eq. (87). In the simplest case of 2HDM, the r_μ variables are $2r_0 = |\phi_1|^2 + |\phi_2|^2$, $2r_3 = |\phi_1|^2 - |\phi_2|^2$, $r_1 = \text{Re}(\phi_1^\dagger \phi_2)$ and $r_2 = \text{Im}(\phi_1^\dagger \phi_2)$, which allow us to write

$$\langle r_0 \rangle^2 - |\langle \mathbf{r} \rangle|^2 = |\langle \phi_1 \rangle|^2 |\langle \phi_2 \rangle|^2 - [\text{Re}(\phi_1^\dagger \phi_2)]^2 - [\text{Im}(\phi_1^\dagger \phi_2)]^2. \quad (48)$$

Notice that the first two terms are custodial invariants while the third is not (20). The latter, $\text{Im}(\phi_1^\dagger \phi_2) = \langle z_{12}^3 \rangle \neq 0$, signals SCPV in the real basis. Therefore, if a potential minimum obeys $\langle r_0 \rangle^2 - |\langle \mathbf{r} \rangle|^2 = 0$ but $\text{Im}(\phi_1^\dagger \phi_2) \neq 0$, one can use $SU(2)_R$ to rotate $\langle \mathbf{z}_{12} \rangle$ in (21) to decrease the 3-component and then increase $\langle r_0 \rangle^2 - |\langle \mathbf{r} \rangle|^2$ in a $SO(4)_C$ -invariant manner.

If we recall the identity (28) for $(cd) = (ab) = (12)$,

$$|\mathbf{z}_{12}|^2 = |\phi_1|^2 |\phi_2|^2 - \text{Re}^2(\phi_1^\dagger \phi_2), \quad (49)$$

one can see that

$$|\langle \mathbf{z}_{12} \rangle|^2 = 0 \quad (50)$$

signals a neutral and CP-invariant vacuum in a custodial-invariant manner. In this case, the first two terms and the third term in Eq. (48) are independently null.

The generalization of Eq. (50) to NHDM is given by

$$\sum_{a < b} |\langle \mathbf{z}_{ab} \rangle|^2 = 0. \quad (51)$$

This condition ensures the symmetry-breaking pattern $SO(4)_C \rightarrow SO(3)_C$.

If the symmetry-breaking pattern $SO(4)_C \rightarrow SO(3)_C$ is realized in a NHDM potential, the residual symmetry $SO(3)_C$ guarantees that all the VEVs of the doublets are aligned as

$$\langle \Phi_a \rangle = v_a \mathbb{1}, \quad a = 1, 2, \dots, N, \quad (52)$$

restricted by

$$2 \sum_a v_a^2 = v_L^2, \quad (53)$$

with $v_L \sim 246 \text{ GeV}$ from successful EWSB. The residual symmetry also guarantees that spontaneous CP violation is not possible.

It is important to emphasize that the degeneracy between CB and CPB vacua happens at tree level. Radiative corrections coming from the gauge sector and the Yukawa sector may break the degeneracy in the effective potential due to interactions that are not $SO(4)_C$ symmetric. Such tree-level degeneracy is a consequence of the symmetry-breaking pattern $SO(4)_C \rightarrow SO(2)_C$ which generates 5 Goldstone bosons. If the low-lying vacuum, after radiative corrections, is neutral and then CPB, three of them will be absorbed as the longitudinal components of the massive

gauge fields. The remaining two scalars will combine to form a charged pseudo-Goldstone boson [28] that acquires a small mass due to radiative corrections [27]. The same is true for any NHDM potential with only two nonzero VEVs that can be reduced to (39) and (40). We are not interested in such a scenario due to the absence of the custodial symmetry that protects the ρ parameter and the lightness of such charged pseudo-Goldstone boson.

The other scenario, i.e., the 2HDM scenario with a low-lying CB vacuum (with radiative corrections) or a NHDM, with $N \geq 3$, with a third doublet with nonzero VEV obeying Eq. (41) (tree-level), has no $U(1)_{em}$ symmetry and contains one more would-be Goldstone boson that gives the photon a mass through the Higgs mechanism. This possibility is thus phenomenologically excluded.

The actual parameter space that avoids the possibility of realizing $\varphi \neq 0, \pi$ in Eq. (40) or $\langle \eta_1^{(3)} \rangle \neq 0$ in Eq. (41) for the global minimum can only be mapped by constructing and analyzing the potential. For a 2HDM custodial-invariant potential with additional Z_2 symmetry, $\phi_2 \rightarrow -\phi_2$, both $SO(4)_C \rightarrow SO(3)_C$ and $SO(4)_C \rightarrow SO(2)_C$ symmetry-breaking patterns are realizable and the explicit parameter ranges for them can be found in Refs. [2, 27].

C. Basis transformation

Since the N Higgs-doublets have the same gauge quantum numbers, any unitary change of basis will maintain the form of the kinetic terms and gauge interactions for the doublets but may modify the form of the potential as well as the Yukawa interactions without changing the physical content of the theory. It amounts to a reparametrization of the potential and Yukawa coefficients.

The most general set of unitary transformations that commutes with the gauge group $SU(2)_L \otimes U(1)_Y$ is given by the basis transformations

$$\phi_a \rightarrow U_{ab}^H \phi_b, \quad U^H \in SU(N)_H. \quad (54)$$

We are already factoring out the global $U(1)$ factor because it corresponds to $U(1)_Y$ transformations.

We can equally write the basis transformation law (54) for Φ_a (1) as [32]

$$\begin{aligned} \Phi_a &\rightarrow (U_{ab}^{H*} \tilde{\phi}_b | U_{ac}^H \phi_c) \\ &= \text{Re}(U_{ab}^H) \Phi_b + \text{Im}(U_{ab}^H) \bar{\Phi}_b \end{aligned} \quad (55)$$

where

$$\bar{\Phi}_a \equiv i(-\tilde{\phi}_a | \phi_a) = \Phi_a(-i)\sigma_3. \quad (56)$$

Notice $\tilde{\Phi}_a = \bar{\Phi}_a$ under (2). If U^H is a complex transformation, it is clear that linear combinations of $\{\phi_a\}$ in the horizontal space of doublets will correspond to linear combinations of $\{\Phi_a\}$ and $\{\bar{\Phi}_a\}$, i.e., only the set $\{\Phi_a\}$ is not sufficient. From the definition (56) we see that a complex basis transformation implicitly induces a transformation in $SU(2)_R$ and it shows that $SU(N)_H$ is not independent of $SU(2)_R$. The transformation law for $\eta^{(a)}$ can be easily extracted from Eq. (55).

As extensively discussed [13, 17, 29], basis transformations might conceal the presence of symmetries by changing how a symmetry acts. That is the case of CP symmetry for example [13, 14, 17]. That is also the case of the canonical implementation (4) of the custodial group $SO(4)_C$. Hence, it is important to study how the representation (4) of the custodial group $SO(4)_C$ is viewed in other bases connected by (54).

To that end, it is useful if we use a representation space where all the groups in question, i.e., $SO(4)_C$ and $SU(N)_H$, act linearly through one matricial representation. It is better to treat $SO(4)_C$ as in (11).

If we define a complex column vector of size $4N$ (it lives in a $4N$ -dimensional *real* vector space) by

$$\chi \equiv \begin{pmatrix} \phi \\ \tilde{\phi} \end{pmatrix}, \quad (57)$$

where

$$\phi \equiv \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{pmatrix}, \quad (58)$$

the canonical representation (11) of $SU(2)_L \otimes SU(2)_R$ translates into

$$\chi \rightarrow (U_R \otimes \mathbb{1}_N \otimes U_L) \chi. \quad (59)$$

Notice $\tilde{\phi}$ in Eq. (57) denotes the application of the tilde operation on each doublet of ϕ in Eq. (58).

If we define new Higgs-doublets ϕ' related by a change of basis (54),

$$\phi = U_1 \phi', \quad \tilde{\phi} = U_1^* \tilde{\phi}', \quad (60)$$

we can see the canonical representation (59) changes into

$$\begin{pmatrix} \phi' \\ -\tilde{\phi}' \end{pmatrix} \rightarrow \begin{pmatrix} U_1^\dagger & \\ & U_1^\top \end{pmatrix} (U_R \otimes \mathbb{1}_N \otimes U_L) \begin{pmatrix} U_1 & \\ & U_1^* \end{pmatrix} \begin{pmatrix} \phi' \\ -\tilde{\phi}' \end{pmatrix}. \quad (61)$$

We can see the representations of $SU(2)_L$ is not modified and we will omit such factor within this analysis. The change in the representation of $SU(2)_R$ can be completely specified if we know the new representation of its generators $\{T'_{kR}\}$:

$$T'_{kR} = \begin{pmatrix} U_1^\dagger & \\ & U_1^\top \end{pmatrix} T_{kR} \begin{pmatrix} U_1 & \\ & U_1^* \end{pmatrix}, \quad k = 1, 2, 3. \quad (62)$$

Obviously $T_{kR} = \frac{1}{2} \sigma_k \otimes \mathbb{1}_N$ for the canonical implementation and we obtain explicitly

$$\begin{aligned} T'_{1R} &= \frac{1}{2} \begin{pmatrix} 0 & U^\dagger \\ U & 0 \end{pmatrix} \\ T'_{2R} &= \frac{1}{2} \begin{pmatrix} 0 & -iU^\dagger \\ iU & 0 \end{pmatrix} \\ T'_{3R} &= \frac{1}{2} \sigma_3 \otimes \mathbb{1}_N = T_{3R}, \end{aligned} \quad (63)$$

where

$$U = U_1^\top U_1. \quad (64)$$

As expected, the representation of $T_{3R} \sim \frac{1}{2} Y$ is not modified since the basis transformations (54) preserve the gauge structure. Only the representation of the generators T_{1R}, T_{2R} of the coset space $SU(2)_R/U(1)_Y$ is modified.

We can also note that the representation for $SU(2)_R$ will be modified only when U_1 in Eq. (60) is complex. In fact, if we restrict the basis transformation group $SU(N)_H$ to $SO(N)_H$, U_1 is orthogonal, $U = \mathbb{1}_N$ in Eq. (64) and the (representation of) generators (63) are the canonical ones. The converse is also true: the only subgroup of $SU(N)_H$ which preserves the representation of $SU(2)_R$ in Eq. (63) is the group of matrices U_1 obeying $U_1^\top U_1 = \mathbb{1}_N$, which is equivalent to $U_1^* = U_1$, i.e., they form the real subgroup $SO(N)_H$. This fact is also in accordance with Eq. (60) which can be rewritten as $\chi_a = (U_1)_{ab} \chi'_b$ for $U_1 \in SO(N)_H$. Hence, there are infinitely many canonical implementations of the custodial group $SO(4)_C$ related by $SO(N)_H$.

We can interpret the previous fact as the realization that *only the real $SO(N)_H$ subgroup of the basis transformation group $SU(N)_H$ commutes with the custodial group $SO(4)_C$* . This also means that the whole global symmetry of the potential can still be enlarged by discrete or continuous subgroups of $SO(N)_H$ without affecting the custodial group.

D. Equivalence among different implementations

We will show in this section the following: *Any implementation of the custodial group $SU(2)_L \otimes SU(2)_R/Z_2$ on a potential containing N Higgs-doublets corresponds to a canonical implementation (4) in some basis provided that*

1. the Higgs kinetic term is invariant by the custodial group;
2. the association $T_{3R} = \frac{1}{2} Y$ fix $U(1)_Y \subset SU(2)_R$;
3. $SU(2)_R$ acts through a reducible representation of N copies of the fundamental **2**-representation.

We already analyzed the converse in Sec. II C, i.e., a canonical implementation of the custodial symmetry satisfies conditions 1, 2 and 3 in any basis.

To prove the statement, we begin by considering χ in Eq. (57) as the appropriate representation space of the N Higgs-doublets ϕ_a . It has the same degrees of freedom of considering the real and imaginary parts of each component of each doublet as independent ($4N$ real fields). Then we note that the representation of $SU(2)_L$ is fixed by the

gauge interactions and each doublet ϕ_a transforms according to the same fundamental representation **2**. If U_L is one element of $SU(2)_L$ in the fundamental representation, it acts reducibly on χ as

$$\chi \xrightarrow{SU(2)_L} (\mathbb{1}_{2N} \otimes U_L) \chi. \quad (65)$$

The action above defines the explicit representation $D(U_L) = \mathbb{1}_{2N} \otimes U_L$.

For the $SU(2)_R$ factor, we want the representation $D(U_R)$ of $U_R \in SU(2)_R$ to commute with any $U_L \in SU(2)_L$, i.e., $[D(U_L), D(U_R)] = 0$ for any U_L, U_R . From the irreducibility of **2** of $SU(2)_L$, the only possibility of the action of $SU(2)_R$ is

$$\chi \xrightarrow{SU(2)_R} (D^{(2N)}(U_R) \otimes \mathbb{1}_2) \chi. \quad (66)$$

We need to specify the representation $D^{(2N)}(U_R)$ in the representation $D(U_R) = D^{(2N)}(U_R) \otimes \mathbb{1}_2$. The following consistency condition should be additionally imposed on such representation in a later stage:

$$(\epsilon \otimes \mathbb{1}_N \otimes \epsilon) \chi^* = \chi. \quad (67)$$

For the $SU(2)_L$ factor the condition above is automatic. Note that Eq. (67) means that complex conjugation acts as a linear transformation on χ .

We begin now to impose condition (1), which requires the form-invariance of the Higgs kinetic term

$$\partial_\mu \phi^\dagger \partial^\mu \phi = \frac{1}{2} \partial_\mu \chi^\dagger \partial^\mu \chi, \quad (68)$$

under the global symmetry $SU(2)_L \otimes SU(2)_R$. The invariance under $SU(2)_L$ is automatic. The invariance under $SU(2)_R$ implies the representation $D^{(2N)}$ should be unitary, i.e.,

$$(D^{(2N)}(U_R))^\dagger D^{(2N)}(U_R) = \mathbb{1}_{2N}, \quad \text{for all } U_R \in SU(2)_R. \quad (69)$$

Recall that any $SU(2)$ representation is equivalent to a unitary representation because it is a compact Lie group.

The representation $D^{(2N)}$ of the Lie group $SU(2)_R$ also induces a representation of the respective Lie algebra $su(2)_R$ through the exponential mapping. The unitarity of $D^{(2N)}$ for $SU(2)$ then induces a Hermitian representation for $su(2)$. We can then work on the group and the algebra interchangeably if we are only interested in the connected part of the group modulo the center. We know $su(2)$ is a three-dimensional Lie algebra and the Pauli matrices $\tau_k \equiv \frac{1}{2} \sigma_k$, $k = 1, 2, 3$, can be used as a basis of the $su(2)$ abstract Lie algebra obeying $[\tau_i, \tau_j] = i\epsilon_{ijk} \tau_k$. We can also regard the explicit form of $\{\tau_k\}$ as the basis for $su(2)$ in the fundamental representation. Using the basis $\{\tau_k\}$, a general element in the $su(2)$ real algebra can be written as $\tau_k a_k$, where a_k , $k = 1, 2, 3$, are real coefficients. The exponential mapping then reads

$$U_R = \exp(i\tau_k a_k), \quad D^{(2N)}(U_R) = \exp(D^{(2N)}(i\tau_k a_k)). \quad (70)$$

We want to embed $U(1)_Y$ into $SU(2)_R$ by requiring condition (2), i.e., by associating hypercharge to the unique diagonal generator of $SU(2)_R$: $T_{3R} = \frac{1}{2}Y$. The action of hypercharge is fixed by the gauge quantum number assignments

$$\chi \xrightarrow{U(1)_Y} e^{i\theta \frac{1}{2}Y} \chi = (e^{i\theta \tau_3} \otimes \mathbb{1}_N \otimes \mathbb{1}_2) \chi. \quad (71)$$

Thus, within the N -Higgs-doublet sector, we obtain

$$T_{3R} = \tau_3 \otimes \mathbb{1}_N \otimes \mathbb{1}_2. \quad (72)$$

and

$$D^{(2N)}(\tau_3) = \tau_3 \otimes \mathbb{1}_N. \quad (73)$$

Now we can identify $U(1)_Y \sim U(1)_{T_{3R}}$. Notice we could have associated $T_{3R} = -Y/2$ and this would only change Eq. (73) to $D^{(2N)}(\tau_3) = -\tau_3 \otimes \mathbb{1}_N$, and the rest of the generators of $SU(2)_R$ accordingly.

We also know all the representations of $SU(2)_R$ are totally reducible and our requirement (3) of the presence of N irreducible **2**-representations implies that there is a $2N \times 2N$ nonsingular matrix U' for which

$$U'^{-1} D^{(2N)}(U_R) U' = U_R \otimes \mathbb{1}_N, \quad \text{for all } U_R \in SU(2)_R. \quad (74)$$

In the algebra Eq. (74) translates into

$$U'^{-1} D^{(2N)}(\tau_k) U' = \tau_k \otimes \mathbb{1}_N, \quad \text{for } k = 1, 2, 3. \quad (75)$$

Notice the usual block diagonal form (direct sum) of N copies of irreducible **2**-representations for τ_k is $\mathbb{1}_N \otimes \tau_k = \text{diag}(\tau_k, \tau_k, \dots, \tau_k)$. But the latter can be transformed into the form (75) by a similarity transformation.

Now, by using Eqs. (73) and Eq. (75), we obtain the condition

$$[U', \tau_3 \otimes \mathbb{1}_N] = 0. \quad (76)$$

Since $\tau_3 \otimes \mathbb{1}_N$ is already diagonal, U' has to have a block diagonal form, each block corresponding to distinct eigenvalues of $\tau_3 \otimes \mathbb{1}_N$

$$U' = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix}. \quad (77)$$

The matrices U_1, U_2 are nonsingular complex matrices of size $N \times N$. Additionally, the unitarity of the representation $D^{(2N)}$ (69) or the hermiticity of (75) implies U_1, U_2 have to be unitary matrices.

The consistency condition (67) yields

$$(\epsilon \otimes \mathbb{1}_N) (D^{(2N)}(U_R))^* (\epsilon \otimes \mathbb{1}_N)^\dagger = D^{(2N)}(U_R). \quad (78)$$

By using (77) we can rewrite

$$\begin{aligned} & \begin{pmatrix} 0 & -\mathbb{1}_N \\ \mathbb{1}_N & 0 \end{pmatrix} \begin{pmatrix} U_1^* & 0 \\ 0 & U_2^* \end{pmatrix} (U_R^* \otimes \mathbb{1}_N) \begin{pmatrix} U_1^\top & 0 \\ 0 & U_2^\top \end{pmatrix} \begin{pmatrix} 0 & \mathbb{1}_N \\ -\mathbb{1}_N & 0 \end{pmatrix} \\ &= \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix} (U_R \otimes \mathbb{1}_N) \begin{pmatrix} U_1^\dagger & 0 \\ 0 & U_2^\dagger \end{pmatrix}, \end{aligned} \quad (79)$$

which reduces to

$$\begin{pmatrix} U_2^\top U_1 & 0 \\ 0 & U_1^\top U_2 \end{pmatrix} (U_R \otimes \mathbb{1}_N) = (U_R \otimes \mathbb{1}_N) \begin{pmatrix} U_2^\top U_1 & 0 \\ 0 & U_1^\top U_2 \end{pmatrix}. \quad (80)$$

The identity (5) was assumed.

Since the previous identity has to be true for the algebra as well, we can use $U_R \rightarrow i\tau_1$ from which we conclude that

$$U_1^\top U_2 = U_2^\top U_1. \quad (81)$$

The same condition arises from $U_R \rightarrow i\tau_2$. The i -factor in $i\tau_1, i\tau_2$ should be present to preserve the condition (67), which should be valid in the group representation but the latter is related to the representation of the algebra by the relation (70).

The explicit representation for τ_k (75) is then

$$\begin{aligned} D^{(2N)}(\tau_1) &= \frac{1}{2} \begin{pmatrix} 0 & U^\dagger \\ U & 0 \end{pmatrix} \\ D^{(2N)}(\tau_2) &= \frac{1}{2} \begin{pmatrix} 0 & -iU^\dagger \\ iU & 0 \end{pmatrix} \\ D^{(2N)}(\tau_3) &= \tau_3 \otimes \mathbb{1}_N \end{aligned} \quad (82)$$

where

$$U = U_2 U_1^\dagger. \quad (83)$$

Notice the matrices in Eq. (82) represent appropriately the algebra $[\tau_i, \tau_j] = i\epsilon_{ijk} \tau_k$.

We can check U is symmetric by using (81)

$$U^\top = U_1^* U_2^\top = U_1^* U_1^\top U_2 U_1^\dagger = U. \quad (84)$$

If we compare Eq. (82) to Eq. (63), we conclude immediately that the matrices in Eq. (82) correspond to the generators of $SU(2)_R$ implemented in some basis $\phi' = U_4^\dagger \phi$. The unitary basis transformation matrix U_4 should satisfy

$$U_4^\top U_4 = U, \quad (85)$$

where U is given by (83). It was shown in Ref. 14 (Appendix B) that the decomposition (85) is always possible for a unitary symmetric matrix U . Thus, there is always a basis for which any implementation of the custodial group obeying the requirements 1, 2 and 3 can be cast into the canonical form (4).

E. Custodial-invariant potential in the canonical form

In this section we want to analyze the most general NHDM potential invariant by the custodial group $SO(4)_C$ in the canonical implementation (CI) and seek general features. Since any implementation of $SO(4)_C$ is equivalent to the CI in some basis, one can always use the latter basis to treat the potential. There are infinitely many such bases.

We begin by writing the most general renormalizable NHDM as [17, 18]

$$V = M_\mu r_\mu + \Lambda_{\mu\nu} r_\mu r_\nu, \quad (86)$$

where r_μ are variables that depend bilinearly on the fields (doublets) and $\{M_\mu, \Lambda_{\mu\nu}\}$ are coefficients. The convention of summation of repeated indices is implicit with Euclidean metric instead of the Minkowski metric used in Ref. 17. In this way, all the indices referring to the variables r_μ will be written as lower indices.

The variables r_μ are defined as [17, 18]

$$r_\mu \equiv (T_\mu)_{ab} \phi_a^\dagger \phi_b, \quad \mu = 0, 1, \dots, d. \quad (87)$$

The $N \times N$ matrices T_μ are

$$T_0 \equiv \sqrt{\frac{N-1}{2N}} \mathbb{1}_N, \quad T_i \equiv \frac{1}{2} \lambda_i, \quad (88)$$

where $\{\lambda_i\}$ are the $d = N^2 - 1$ hermitian generators of $SU(N)_H$ in the fundamental representation, obeying the normalization $\text{Tr}[\lambda_i \lambda_j] = 2\delta_{ij}$.

We can choose $\{T_i\}$ to be the generalization of the Gell-Mann matrices of $SU(3)$ to $SU(N)$. We separate them into three classes: diagonal matrices $\{h_i\}$, off-diagonal symmetric matrices $\{\mathcal{S}_{ab}\}$, and off-diagonal antisymmetric matrices $\{\mathcal{A}_{ab}\}$, with r, q, q elements, respectively [$r = N - 1$, $q = \frac{1}{2}N(N - 1)$]. The matrices $\{h_i\}$ correspond to a basis for the Cartan subalgebra while the \mathcal{S}_{ab} and \mathcal{A}_{ab} correspond to the symmetric and antisymmetric combinations of ladder operators labeled by the pair (ab) , $a < b$, $a, b = 1, \dots, N$. More explicitly, we can write

$$\mathcal{S}_{ab} = \frac{1}{2}(e_{ab} + e_{ba}) \quad \text{and} \quad \mathcal{A}_{ab} = \frac{1}{2i}(e_{ab} - e_{ba}), \quad (89)$$

where e_{ab} are the canonical matrices obeying $(e_{ab})_{ij} = \delta_{ai}\delta_{bj}$. We can follow, for instance, the ordering

$$(ab) = (12), (23), \dots, (N-1, N), (13), \dots, (N-2, N), \dots, (1, N). \quad (90)$$

For example, for $SU(3)$ we would have $\{h_1, h_2\} = \{\lambda_3/2, \lambda_8/2\}$, $\{\mathcal{S}_{12}, \mathcal{S}_{23}, \mathcal{S}_{13}\} = \{\lambda_1/2, \lambda_6/2, \lambda_4/2\}$ and $\{\mathcal{A}_{12}, \mathcal{A}_{23}, \mathcal{A}_{13}\} = \{\lambda_2/2, \lambda_7/2, \lambda_5/2\}$. The ordering (90) follows the ordering of the lower to higher heights of the roots and the first r of them correspond to the simple roots.

We will denote the variables r_μ corresponding to $\{h_i, \mathcal{S}_{ab}, \mathcal{A}_{ab}\}$ respectively by

$$\{r_{(i)}, r_{(ab)}, r_{(\overline{ab})}\}. \quad (91)$$

Therefore $\{r_{(i)}\}$ are combinations of $\phi_a^\dagger \phi_a$ while

$$r_{(ab)} = \text{Re}(\phi_a^\dagger \phi_b), \quad r_{(\overline{ab})} = \text{Im}(\phi_a^\dagger \phi_b), \quad a < b. \quad (92)$$

Then the elimination of the terms (23) and (24) corresponds in Eq. (86) to

$$M_\mu = 0 \quad \text{for } \mu = (\overline{ab}) \quad (93)$$

and

$$\Lambda_{\mu\nu} = 0 \quad \text{for } \mu = (\overline{ab}) \text{ or } \nu = (\overline{ab}), \quad (94)$$

where *or* means one of them exclusively. The restriction (94) leads to the block diagonal form for the $d \times d$ submatrix $\tilde{\Lambda} = (\Lambda_{ij})$:

$$\tilde{\Lambda} = \begin{pmatrix} A_{p \times p} & 0_{p \times q} \\ 0_{q \times p} & B_{q \times q} \end{pmatrix}, \quad (95)$$

where $p \equiv r + q = N(N + 1)/2$ and $0_{p \times q}$ denotes the null matrix of the shown dimension.

For $N \leq 3$, we have to impose additionally

$$\Lambda_{\mu\nu} = 0 \quad \text{for } \mu = (\overline{ab}) \text{ and } \nu = (\overline{ab}). \quad (96)$$

The restriction (96) sets $B_{q \times q} = 0_{q \times q}$ in Eq. (95). The most general custodial invariant 2HDM and 3HDM potentials are then given by (86) with the restrictions (93), (94) and (96):

$$V = \sum_{\mu=0, (i), (ab)} M_{\mu} r_{\mu} + \sum_{\mu, \nu=0, (i), (ab)} \Lambda_{\mu\nu} r_{\mu} r_{\nu}, \quad (97)$$

where the summation is explicitly shown.

In this case, we can confirm the direct connection between the presence of *only one charged would-be Goldstone boson* and a *CP-conserving vacuum*. Such connection follows from the complete absence of the terms $\text{Im}(\phi_a^{\dagger} \phi_b)$ in the potential (97), from which we immediately conclude that independently of r_{μ} ,

$$\frac{\partial V}{\partial r_{(\overline{ab})}} = 0, \quad a < b = 1, \dots, N. \quad (98)$$

Therefore, we can immediately write the extremum equations as [18]

$$\frac{\partial V}{\partial \phi_{ai}} = (\mathbb{M})_{ab} \phi_{bi} = \sum_{\mu=0, (i), (cd)} \frac{\partial V}{\partial r_{\mu}} (T_{\mu})_{ab} \phi_{bi}. \quad (99)$$

We know $\langle \mathbb{M} \rangle$, the matrix \mathbb{M} computed for the minimal values (VEVs), is the squared-mass matrix for the charged scalars for a neutral vacuum [18], including the charged Goldstone bosons. If there is only one (would-be) charged Goldstone boson, then the VEVs corresponding to the second components of each doublet, $\langle w_a \rangle = \langle \phi_{a2} \rangle$, form the unique eigenvector of $\langle \mathbb{M} \rangle$ associated with the null eigenvalue. We can see from Eq. (99) that \mathbb{M} is real and symmetric because the sum only contains generators T_{μ} that are real and symmetric. Since the eigenvalues of $\langle \mathbb{M} \rangle$ have to be real, the eigenvector $\langle w \rangle$ is also real and then spontaneous CP violation is excluded [33]. Obviously, this happens because we are implicitly selecting the symmetry-breaking pattern $SO(4)_C \rightarrow SO(3)_C$. The direct connection above, however, is not apparent for custodial-invariant NHDM potentials with $N \geq 4$.

The independence of the potential on any $r_{(\overline{ab})}$ (98) also explains why CB and SCPV vacua are degenerate for the custodial-invariant 2HDM. In this case, the potential does not depend on r_2 , which can be changed continuously and independently in that direction (within the surface and interior of the lightcone in Ref. [21]) without changing the potential value. The physical range of the variables r_{μ} (87) in the 2HDM corresponds to all the points inside and on the surface of a cone (lightcone) defined by $r_0^2 - \mathbf{r}^2 = 0$, where $\mathbf{r}^2 = r_1^2 + r_2^2 + r_3^2$. The VEVs lying on the surface of such a cone correspond to neutral vacua while the interior points correspond to charge-breaking vacua. Then, if there is a neutral but CP-violating vacuum $\langle r_{\mu} \rangle$ obeying $\langle r_0^2 - \mathbf{r}^2 \rangle = 0$, with $\langle r_2 \rangle \neq 0$, the vacuum with the same values of r_0, r_1, r_3 but $\langle r_2 \rangle = 0$ lies at the same depth of the potential but it is charge breaking since $\langle r_0^2 - \mathbf{r}^2 \rangle > 0$. The same conclusion can be reached for 3HDM if we can find independent directions to move in the subspace of r_2, r_5, r_7 in the orbit space [19].

For $N \geq 4$, the most general custodial invariant NHDM potentials are obtained by adding to (97) the term

$$\Delta V_4 = \sum_{a < b < c < d} \lambda_{abcd} I_{abcd}^{(4)}. \quad (100)$$

From the definition of $I^{(4)}$ (34) we can establish the correspondence

$$\lambda_{abcd} = 2\Lambda_{(\overline{ab})(\overline{cd})} = -2\Lambda_{(\overline{ac})(\overline{bd})} = 2\Lambda_{(\overline{ad})(\overline{bc})}, \quad (101)$$

for $a < b < c < d$. Equation (101) restricts $\Lambda_{\mu\nu}$ for $\mu, \nu = (\overline{ab})$. For $N = 4$, the expression (100) contains only one term $I_{1234}^{(4)}$.

Notice that for $N \geq 4$, Eq. (98) is not valid. Because of Eqs. (100) and (101), however, the coefficients $\Lambda_{\mu\nu}$ in the sector of $r_{(\overline{ab})} r_{(\overline{cd})}$ is a sparse matrix. For example, for $N = 4$, in the subspace of $\{r_{(\overline{12})}, r_{(\overline{13})}, r_{(\overline{14})}, r_{(\overline{23})}, r_{(\overline{24})}, r_{(\overline{34})}\}$, the submatrix $B_{q \times q}$ in Eq. (95) can be written as

$$B_{6 \times 6} = \left(\Lambda_{(\overline{ab})(\overline{cd})} \right) = \lambda_{1234} \begin{pmatrix} 0_{3 \times 3} & B_1 \\ B_1 & 0_{3 \times 3} \end{pmatrix},$$

$$B_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \quad (102)$$

It is clear that the block matrix in Eq.(102) has eigenvalues $\pm\lambda_{1234}$, each one with multiplicity 3. The explicit construction for $N = 5$, reveals that the corresponding block matrix has eigenvalues $0, \lambda, -\lambda$, with multiplicities 4, 3, 3, respectively, where λ is a positive number that depends on the 5 parameters λ_{abcd} , $a < b < c < d$.

III. DIFFERENT IMPLEMENTATIONS IN 2HDM

We analyze in the following the different, but equivalent, implementations of $SO(4)_C$ in the 2HDM potential. The first two implementations, Secs.III A and III B, were already considered in the literature but we show in Sec.III C that they can be generalized.

A. Twisted implementation

It can immediately be seen that the “twisted” implementation of the custodial symmetry in Ref.23 is just the canonical symmetry (4) imposed in a basis

$$\phi'_a = e^{i\theta_a} \phi_a, \quad a = 1, 2. \quad (103)$$

It corresponds to a change of basis in Eq.(60) with

$$U_1^\dagger = \text{diag}(e^{i\theta_a}), \quad (104)$$

where we can choose $\sum_a \theta_a = 0$ from $U(1)_Y$ invariance.

This implementation can be straightforwardly generalized to N -Higgs-doublets with general $N \geq 2$.

For the particular case of 2HDM, two apparently inequivalent implementations of the custodial group were presented in Ref. 23. The twisted version was shown to allow for the degeneracy between the charged Higgs H^\pm and the CP-even scalar H^0 , $M_{H^0} = M_{H^\pm}$. However, as shown in Sec.II D, any implementation of the custodial group is equivalent to the canonical one in some basis. In the specific case of the twisted version of Ref.23, the required change of basis is the rephasing transformation of (103). After the appropriate basis change, the canonical CP transformations automatically constitute a symmetry of the Higgs potential. Let us call such automatic symmetry CP1. Thus the “twisted” implementation corresponds to an imposition of an additional CP2 symmetry, orthogonal to CP1 in the sense of Ref. 17, apart from the automatic CP1 symmetry. With respect to the CP1 symmetry, the CP2-even scalar H^0 is actually CP1-odd. Obviously, one can choose one of the CP symmetries to be a true symmetry of the theory by extending it to the Yukawa sector. Only then, is it possible to define (approximately) the scalar degenerate to H^\pm as CP-even, the CP symmetry being the CP2 transformation. A similar comment has been already made in Ref. 24.

B. Type II implementation

For the specific case of the 2HDM, various apparently different implementations of the custodial group can be devised. An implementation called type II [22] follows from the action of $SU(2)_L \otimes SU(2)_R$ upon

$$M_{12} \equiv (\tilde{\phi}_2 | \phi_1), \quad (105)$$

instead of the action on Φ_1, Φ_2 . This implementation was first considered in Ref. 22 as distinct from the canonical one, which was named type I. However, Refs. [24, 25] show that they are in fact equivalent to a canonical implementation in a different basis.

To complement such discussion, let us analyze the equivalence between type II and canonical implementation from a slightly different perspective.

The matrix M_{12} is a general complex 2×2 matrix, different from Φ_a which obeys (3). In terms of independent degrees of freedom (real fields), Φ_1 and Φ_2 together has 8 degrees of freedom, the same number as for M_{12} . The action of $SU(2)_L \otimes SU(2)_R$ on M_{12} in Eq.(105) is, however, reducible because of the property (5). The irreducible pieces of M_{12} can be separated, respectively, as the even and odd parts under the tilde operation (2):

$$M_{12}^{(+)} = \frac{M_{12} + \tilde{M}_{12}}{\sqrt{2}},$$

$$M_{12}^{(-)} = \frac{M_{12} - \tilde{M}_{12}}{\sqrt{2}}. \quad (106)$$

We can also think the tilde operation as a linear transformation in the space of χ_a (10) with two eigenvalues, ± 1 , that separates the irreducible representations of M_{12} .

In other words, we can define doublets ϕ'_1 and ϕ'_2 associated, respectively, to

$$\begin{aligned} \Phi'_1 &\equiv M_{12}^{(+)} = a_\mu \mathbf{e}_\mu, \\ \Phi'_2 &\equiv -iM_{12}^{(-)} = b_\mu \mathbf{e}_\mu. \end{aligned} \quad (107)$$

or, equivalently,

$$M_{12} = \frac{1}{\sqrt{2}}(a_\mu + ib_\mu)\mathbf{e}_\mu, \quad (108)$$

where a_μ and b_μ are 4-vectors similar to $\eta^{(a)}$. The explicit relation between the doublets ϕ_a in (105) and ϕ'_a is given by

$$\begin{aligned} \phi'_1 &= \frac{\phi_1 + \phi_2}{\sqrt{2}}, \\ \phi'_2 &= \frac{\phi_1 - \phi_2}{\sqrt{2}i}. \end{aligned} \quad (109)$$

One can see, as expected, that the type II implementation on (105) corresponds to the canonical implementation on ϕ'_a through Φ'_a constructed as Eq. (1). It should be remarked that the basis change in Eq. (109) connecting type II implementation and canonical implementation is not unique because any additional $SO(2)_H$ transformation on ϕ'_a still preserves the canonical implementation of $SO(4)_C$.

C. Other implementations

We have shown in Sec. IID that all implementations of the custodial group are equivalent to the canonical implementation in some basis. For the 2HDM potential we can show another practical way of implementing custodial symmetry, in clear analogy with type II implementation, without resorting to basis change.

In this class of implementation we define

$$M_{1'1} \equiv (\tilde{\phi}'_1 | \phi_1), \quad (110)$$

where

$$\phi'_1 = c_1 \phi_1 + c_2 \phi_2, \quad |c_1|^2 + |c_2|^2 = 1. \quad (111)$$

We can easily see $(c_1, c_2) = (1, 0)$ [in this case Φ_2 will be also necessary] and $(c_1, c_2) = (0, 1)$ correspond to the canonical and type II implementations respectively.

The action of $SU(2)_L \otimes SU(2)_R$ is given by

$$M_{1'1} \rightarrow U_L M_{1'1} U_R^\dagger. \quad (112)$$

By analyzing the infinitesimal transformation of $SU(2)_R$ on ϕ_1 and ϕ_2 , we can conclude that such implementation is equivalent to the canonical implementation on (ϕ'_1, ϕ'_2) given by

$$\begin{pmatrix} \phi'_1 \\ \phi'_2 \end{pmatrix} = \begin{pmatrix} c_1 & c_2 \\ c_2 & -\frac{c_1^* c_2}{c_2^*} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \quad (113)$$

One can check the previous transformation matrix is unitary and symmetric.

IV. CONSEQUENCES AND CONCLUSIONS

We have shown in Sec.IID that any implementation of the custodial $SO(4)_C \sim SU(2)_L \otimes SU(2)_R$ group in a NHDM potential is equivalent to the canonical implementation in some basis if $SU(2)_L$ is the gauge factor, $U(1)_Y$ is embedded in $SU(2)_R$, and we require N copies of the doublet representation of $SU(2)_R$. On the other hand, we have seen in Sec.IIA that a potential invariant by $SO(4)_C$ in the canonical implementation (CI) is automatically CP-invariant in its canonical form (CCP). Therefore, *any NHDM potential invariant by a global $SO(4)_C$ symmetry is also automatically CP-symmetric independently of the implementation.* Moreover, the basis for which $SO(4)_C$ implementation is canonical is automatically aligned to the basis where the CP transformation on the doublets is canonical. If one requires the custodial symmetry $SO(3)_C$ to remain after EWSB, spontaneous CP violation is automatically excluded as well.

One can then take advantage of such result to use explicit CP invariance as a necessary criterion to identify global $SO(4)_C$ invariance in a NHDM potential, even if its manifestation is not explicit. Several tools based on basis invariant conditions were already developed for identifying CP-invariance in a general NHDM potential [13, 14, 17]. One can also make use of the fact that a CP-invariant NHDM potential can be always written in the so-called *real basis* (or the canonical CP basis [17]) where all the parameters of the potential written in terms of the gauge invariants $\phi_a^\dagger \phi_b$ are real [14]. In other words, there is always a basis where the CP symmetry manifests canonically (14).

To find such basis for a general CP-invariant NHDM potential with $N \geq 3$ is a difficult technical and unsolved problem [17]. For the 2HDM, the change of basis from a general basis to the real basis can be explicitly given [17]. For the 3HDM, necessary and sufficient criteria for CP invariance can be devised but the systematic method to find the real basis is lacking [17]. In both cases, once we write the CP-invariant potential in its real form, then identifying if the potential is $SO(4)_C$ -symmetric is a straightforward task because any real basis is also a basis where the action of the $SO(4)_C$ symmetry is canonical. Thus, it suffices to check if the potential is entirely written in terms of $\text{Re}(\phi_a^\dagger \phi_b)$ in its linear and quadratic combinations, just as in Eq.(97). Such a criterion is invariant by the residual $SO(3)_H$ reparametrization freedom that remains.

For the specific case of the 2HDM, basis-invariant conditions to test $SO(4)_C$ can be written [25]. If we follow the methods of Ref.17, we can consider the parameters $\{\mathbf{M} = (M_i), \mathbf{\Lambda}_0 = (\Lambda_{0i}), \tilde{\Lambda} = (\Lambda_{ij})\}$ as two vectors and one rank-2 tensor of $SO(3)_H$, respectively. These parameters were defined in Eq.(86). CP transformations then act through ordinary reflection in three dimensions along a direction \mathbf{k}_{CP} called CP-reflection direction, which might not be unique. CP invariance then is equivalent to the existence of \mathbf{k}_{CP} such that

$$\mathbf{k}_{CP} \cdot \mathbf{M} = 0, \quad \mathbf{k}_{CP} \cdot \mathbf{\Lambda}_0 = 0, \quad \mathbf{k}_{CP} \text{ is an eigenvector of } \tilde{\Lambda}. \quad (114)$$

In addition, the potential is $SO(4)_C$ -invariant if, and only if,

$$\mathbf{k}_{CP} \text{ is an eigenvector of } \tilde{\Lambda} \text{ associated to the eigenvalue } 0. \quad (115)$$

Obviously $\det \tilde{\Lambda}$ should be null [25]. The possible directions for \mathbf{k}_{CP} were given in Ref.17 but when $\mathbf{M}, \mathbf{\Lambda}_0$ are not null and nonparallel vectors, $\mathbf{k}_{CP} = \mathbf{M} \times \mathbf{\Lambda}_0$ is certainly one CP-reflection direction.

For 3HDMs, a systematic procedure to find the real basis was not completed but we can still write the necessary and sufficient conditions to have $SO(4)_C$ symmetry. If the potential is CP-symmetric, there should be a three-dimensional CP-odd subspace \mathbf{t}'_q of the adjoint space, the 8-dimensional euclidean space where $\mathbf{r} = (r_i)$ lives, such that [17]

$$\mathbf{M} \perp \mathbf{t}'_q, \quad \mathbf{\Lambda}_0 \perp \mathbf{t}'_q, \quad \mathbf{t}'_q \text{ is an invariant subspace of } \tilde{\Lambda}. \quad (116)$$

In the real basis, \mathbf{t}'_q is spanned by $\{\lambda_2, \lambda_5, \lambda_7\}$. The potential is additionally $SO(4)_C$ -invariant if, and only if,

$$\mathbf{t}'_q \text{ is contained in the nullspace of } \tilde{\Lambda}. \quad (117)$$

For $N \geq 4$, a real basis may not coincide with a basis of CI of $SO(4)_C$. More specifically, CCP invariance (real basis) requires the parameters $\{M_\mu, \Lambda_{\mu\nu}\}$ to obey some but not all of the restrictions for $SO(4)_C$ invariance in the CI. The restrictions for CCP invariance coincide with Eqs. (93), (94) and (95), but $SO(4)_C$ invariance additionally requires that $B_{q \times q}$ in Eq. (95) should be compatible with the structure in Eq. (100).

For example, for $N = 4$, a CP-invariant potential can be brought to the real basis where we can identify the block matrix $B_{q \times q}$ in $(\Lambda_{\mu\nu})$. If the potential is also $SO(4)_C$ -invariant, the structure of $B_{q \times q}$ should be of the form in Eq. (102) (CI) or $SO(4)_H$ equivalent. The group $SO(4)_H$ appears as the real subgroup of the reparametrization group $SU(4)_H$ which preserves the representations of $SO(4)_C$ and in fact it is the only compatible reparametrization group. Now, an element g of the group $SO(4)_H$ acts on $B_{6 \times 6}$ as

$$B_{6 \times 6} \rightarrow D^6(g) B_{6 \times 6} D^{6T}(g), \quad g \in SO(4)_H,$$

where D^6 is the 6-dimensional adjoint representation of g . Certainly, from Eq. (102), $SO(4)_C$ invariance requires $B_{6 \times 6}$ to have only two eigenvalues $\pm\lambda$ with multiplicity 3 each. The problem is that such condition is not sufficient to guarantee that there is a matrix $D^6(g)$ that transform $B_{6 \times 6}$ into the form (102) because a $SO(6)$ orthogonal matrix is necessary in general. Therefore, additional conditions are necessary.

In the same way, we can extract the necessary condition for $N = 5$: $B_{q \times q}$ in the real basis should have eigenvalues $0, \lambda, -\lambda$ with multiplicities 4, 3, 3 respectively. Analogous necessary conditions for general $N \geq 4$ could be found by studying the terms in (100).

As for the general problem of constructing the most general NHDM potential invariant by the global $SO(4)_C$ symmetry, we managed to solve it in its simplest form: we can write the most general custodial-invariant potential before EWSB. The details of EWSB and the parameter range to achieve the desired symmetry-breaking pattern $SO(4)_C \rightarrow SO(3)_C$ will be left for further work. For the Z_2 -symmetric 2HDM, the parameter range is known since Refs. [2, 27].

In any case, we confirmed that the phenomenologically interesting symmetry-breaking pattern is $SO(4)_C \rightarrow SO(3)_C$. In this case, the custodial symmetry $SO(3)_C \sim SU(3)_{L+R}$ remains as an approximate symmetry at the electroweak scale and protects the ρ parameter of acquiring large radiative corrections quadratic in the masses of the scalars.

The other viable $SO(4)_C \rightarrow SO(2)_C$ symmetry-breaking pattern does not have the custodial symmetry and its viability in realistic models can not be treated at tree level because the CP-violating but neutral vacua are degenerate with the charge-breaking vacua. Only if radiative corrections are taken into account, can we check which models have one neutral vacuum lying deeper than the charge-breaking vacua. This fact was not sufficiently emphasized in previous works [24, 25, 27].

Because the symmetry-breaking $SO(4)_C \rightarrow SO(2)_C$ is possible and spontaneously CP-violating and charge-breaking vacua might be degenerate, we can conclude that *the imposition of the custodial group $SO(4)_C$ before EWSB and the requirement of $SO(3)_C$ custodial symmetry are separate conditions in NHDMs* (with $N > 1$). The imposition of the global $SO(4)_C$ symmetry certainly implies explicit CP invariance in the NHDM potential but the possibility of having spontaneous CP violation is still present with the possibility of the pattern $SO(4)_C \rightarrow SO(2)_C$.

An interesting question that arises through the study of the global $SO(4)_C$ in NHDMs is the role played by global symmetries in the potential. For the 2HDM, with Z_2 symmetry, different global symmetries ranging from the usual G_{SM} to $SO(8)$ were studied in Ref. 27. In general, for a global symmetry larger than $SO(4)_C$, (pseudo) Goldstone bosons appear [28]. For example, the global symmetry group $G_{SM} \otimes SU(2)_H$ is broken down to $U(1) \otimes U(1)_{em}$ generating three would-be Goldstone bosons and two true Goldstone bosons associated with the breaking of $SU(2)_H$. These true Goldstone bosons are neutral. Reference [27] also explored the possibilities of having $SO(4)$, $SO(4) \otimes SO(4)$ and $SO(8)$ as global symmetries. The case of the $SO(4)$ group is the usual custodial symmetry extended to 2HDM. The case of $SO(4) \otimes SO(4)$ is the unlocked case where the custodial symmetry acts independently for both doublets. In these cases the global symmetry is not an independent factor but contains the gauge symmetries of the SM. A detailed study of possible approximate symmetries in NHDMs is performed in Ref. 34.

The maximal continuous global symmetry in 2HDMs is $SO(8)$ contained in $O(8)$. In this case, there is no additional continuous symmetry definable and the reparametrization group $SU(2)_H$ is also contained in $SO(8)$. Electroweak symmetry breaking proceeds through only one breaking pattern of the global symmetry: $SO(8)$ into $SO(7)$, where 7 Goldstone bosons emerge, among them some will be absorbed by the Higgs mechanism while the remaining will be pseudo-Goldstone bosons. The gauge interactions respects only G_{SM} . Then, the breaking pattern of the gauge group G_{SM} is not defined at the tree level of the potential because one nontrivial $SO(8)$ orbit contains both VEVs that are neutral and charge breaking with respect to G_{SM} . Radiative corrections of the gauge interactions should be incorporated to decide which model preserves $U(1)_{em}$ and to calculate the radiative masses of the pseudo-Goldstone bosons. The fate of the CP symmetry may depend on the radiative corrections of the gauge sector as well as of the Yukawa sector that violates CP.

Therefore the consideration of $SO(4)_C$ as a global symmetry in NHDMs has two advantages: (i) it can preserve the approximate custodial symmetry $SO(3)_C$ and (ii) it avoids the presence of pseudo-Goldstone bosons and degenerate symmetry breaking patterns at tree level. If we insist on considering only the global $SO(4)_C$ symmetry in NHDMs, the immediate question towards generalization is if we can use different representations n_a other than the doublet representation for $SU(2)_R$. The canonical implementation uses $n_a = 2$ for all ϕ_a . We immediately conclude that the association $Y/2 = T_{3R}$ is not possible for any other representation $n_a > 2$, since we have only two hypercharges, one for ϕ_a and the opposite for ϕ_a^* , common to all the doublets. For example, to have $n_a = 3$ we need a state with zero hypercharge and to have $n_a = 4$, we need two different hypercharges in modulus. Related to that, one can obviously embed the electroweak gauge group into a larger group that is broken at high energies to a model containing two or more Higgs doublets with a global accidental symmetry inherited from the high-scale symmetry [35].

Within the setting of Sec. IID, different but equivalent implementations of $SO(4)_C$ were considered for the 2HDM in the literature. We reviewed them in Sec. III and showed a generalization in Sec. III C. We explicitly showed the basis change necessary to obtain the canonical implementation.

Another interesting general feature of the NHDMs implementing the global $SO(4)_C$ symmetry is the role played by the residual $SO(N)_H$ reparametrization freedom. For $N = 2$, it is just the freedom to rotate the plane perpendicular to \mathbf{k}_{CP} . For $N = 3$, it is the $SO(3)_H$ freedom to reparametrize \mathbf{t}'_q and its orthogonal complement. Such reparametrization freedom can still be used to study general $SO(4)_C$ invariant potentials. Another possible role for $SO(N)_H$ is the possibility to promote the whole group or some subgroup G'_H to symmetries of the potential independently of the $SO(4)_C$ symmetry. The global symmetry in this case would be $SO(4)_C \otimes G'_H$. Obviously, the symmetry G'_H could be broken by EWSB.

It is important to emphasize that the whole horizontal group $SU(N)_H$ in NHDM no longer commutes with the $SO(4)_C$ symmetry and some invariants that are $SU(N)_H$ -invariant may not be $SO(4)_C$ -invariant. That is the case of the invariant $\langle r_0^2 - \mathbf{r}^2 \rangle$ in 2HDM [18, 21] that characterizes neutral vacuum if its null. Since it is not an $SO(4)_C$ invariant, its consideration alone can not distinguish among some symmetry-breaking patterns of the gauge group for the pattern $SO(4)_C \rightarrow SO(2)_C$. A $SO(4)_C$ -invariant measure for $SO(4)_C \rightarrow SO(3)_C$ was shown in Eq. (51).

Another context where basis transformations are important is the connection with the Yukawa sector. Although all the implementations of $SO(4)_C$ symmetry are equivalent within the Higgs potential, some properties of the whole theory (Lagrangian), including symmetries, might depend on how the symmetry is implemented in one sector relative to the other. Since the global $SO(4)_C$ is explicitly broken by the gauge interactions and Yukawa interactions, the breaking effects depend on the implementation of the symmetry in the potential relative to the other breaking sectors [25, 30].

Understanding how the breaking of some global symmetries occurs is also important in other contexts such as flavor physics. For example, Ref. 36 compares the possibility of FCNC in multi-Higgs models under the perspective of the two most popular suppression mechanisms, namely, Natural Flavor Conservation (NFC) and Minimal Flavor Violation (MFV) [37]. It is also possible to constrain 2HDM models from the requirement of mass hierarchy and suppression of FCNC [38].

In summary, we have shown that all implementations of the $SO(4)_C$ global symmetry in NHDMs are equivalent within some general conditions such as the presence of N equal representations of $SU(2)_R$. Such results have enabled us to study a general $SO(4)_C$ -invariant potential in its canonical implementation where the CP symmetry is manifest. We have shown that for $N = 2, 3$ the difference between $SO(4)_C$ -invariant and CP-invariant potentials is minimal and the knowledge of the CP symmetry immediately gives information about $SO(4)_C$ -invariance or violation in the potential. We have explicitly reviewed some implementations for the 2HDM and showed a general implementation.

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Appendix A: Custodial symmetry: SM and notation

The Higgs potential in SM possesses a global accidental $SO(4)_C \sim SU(2)_L \otimes SU(2)_R / Z_2$ symmetry due to the presence of one isolated doublet representation. Such symmetry group contains the electroweak gauge group $G_{SM} \equiv SU(2)_L \otimes U(1)_Y$ as a subgroup, which is the true symmetry of the Higgs Lagrangian, including the gauge interactions.

The electroweak symmetry G_{SM} is then broken down to $U(1)_{em}$ by the Higgs VEV $\langle \phi^0 \rangle$. At the same time, the EWSB mechanism breaks $SO(4)_C$ down to the subgroup $SO(3)_C \sim SU(2)_{L+R}$ containing $U(1)_{em}$, which is the only nontrivial symmetry-breaking pattern possible. In the absence of $U(1)_Y$ interactions ($g_Y \rightarrow 0$ limit), the three would-be Goldstone bosons absorbed by the Higgs mechanism form a triplet under $SO(3)_C$. Such symmetry protects the ρ parameter from large radiative corrections quadratic in the Higgs mass and it is called custodial symmetry [2, 3].

Instead of distinguishing the various symmetries above by names, we denote them by their group structure and use the isomorphic groups interchangeably, often considering their local structure only. The groups in question are

$$\begin{array}{ccc} SU(2)_L \otimes U(1)_Y & \subset & SU(2)_L \otimes SU(2)_R / Z_2 \sim SO(4)_C \\ \downarrow \text{EWSB} & & \downarrow \text{EWSB} \\ U(1)_{em} & \subset & SU(2)_{L+R} \sim SO(3)_C. \end{array} \quad (\text{A1})$$

The subgroup/group relation in the first line of Eq. (A1) also considers $U(1)_Y \subset SU(2)_R$.

Appendix B: Generators of $SO(4)_C$

The transformation matrix \mathcal{B} in (12) is given by

$$\mathcal{B} = \begin{pmatrix} 0 & i & 1 & 0 \\ 1 & 0 & 0 & -i \\ -1 & 0 & 0 & -i \\ 0 & -i & 1 & 0 \end{pmatrix}. \quad (\text{B1})$$

This relation can be read from Eq. (6).

If we define the generators of $SU(2)_{L+R}$ and $SU(2)_{L-R}$ acting on χ_a as

$$\begin{aligned} L_j &\equiv T_{Lj} + T_{Rj} = \mathbb{1}_2 \otimes \frac{\sigma_j}{2} + \frac{\sigma_j}{2} \otimes \mathbb{1}_2 \\ K_j &\equiv T_{Lj} - T_{Rj} = \mathbb{1}_2 \otimes \frac{\sigma_j}{2} - \frac{\sigma_j}{2} \otimes \mathbb{1}_2 \end{aligned} \quad (\text{B2})$$

the generators acting on $\eta^{(a)}$ are

$$\begin{aligned} L'_j &= \mathcal{B}^{-1} L_j \mathcal{B} \\ K'_j &= \mathcal{B}^{-1} K_j \mathcal{B}. \end{aligned} \quad (\text{B3})$$

Or explicitly,

$$\begin{aligned} L'_1 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} & K'_1 &= \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ L'_2 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} & K'_2 &= \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ L'_3 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} & K'_3 &= \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \end{aligned} \quad (\text{B4})$$

We can immediately notice that $\{L_j\}$ are the generators of $SO(3)_C$ and $\{K_j\}$ are the generators of the cosets $SO(4)_C/SO(3)_C$.

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